A CRITERION FOR THE CHOICE OF THE INTERPOLATION KERNEL IN SMOOTHED PARTICLE HYDRODYNAMICS

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Abstract. We study the problem of the appropriate choice of the interpolating kernel to be used in the evaluation of gradients of functions. Such interpolation technique is often used in applications, e.g. it is typical fo Smoothed Particle Hydrodynamics (SPH). We propose a minimization procedure for selecting kernels in $\Re^n$, in the class of regular, normalizable, symmetric functions having finite moments up to a sufficiently high order; the method is valid when the kernel width is position–dependent and allows to recover conservation laws at the same order of approximation that SPH, as interpolation technique, has when the kernel size is constant.

1 Introduction

The aim of this paper is giving a criterion for the choice of kernel functions to be used in a particular interpolation problem. The problem is the fitting of spatial derivatives of a function f (for example the gradient of f, ∇f) known on a finite set of points in $\Re^3$. The results here presented do not depend on the way the points are chosen and valid in fully n–dimensional situations.

The problem of gradient interpolation assumes the form of the right choice of interpolating kernels in the so-called Smoothed Particle Hydrodynamics (SPH) method (we refer to [1] for an introduction to this numerical method and to [2] for some recent improvements). In this scheme the fluid is sampled by a set of massive particles which are "fluid representatives": the particle positions are considered as moving grid-points for the interpolation of the physical quantities characterizing the fluid as well as their spatial derivatives. SPH is so a fully Lagrangian method. Analogously to the classic mollification approximation of a sufficiently regular function f with the convolution function $\langle f \rangle \equiv f * \phi$, where $*$ is the convolution operator and ϕ is a kernel function (whose properties will be specified later), the spatial derivatives of f, resumed by ∇f, are approximated by $\langle \nabla f \rangle_1 \equiv (\nabla f) * \phi$. In doing this, we take the advantage that, under suitable hypotheses on f and ϕ, $(\nabla f) * \phi$ can be replaced by $f * \nabla \phi$. As final step, the integral $f * \nabla \phi$ is numerically evaluated. Note that the knowledge of f on a set of points suffices to evaluate $\langle \nabla f \rangle_1$, and the numerical evaluation of the integral giving $f * \nabla \phi$ can be done using a Monte-Carlo estimate. The interpolation procedure used in SPH follows the scheme we have just sketched, so we shall refer to this scheme as "SPH-like". We start our analysis noting that another approximation for ∇f can be given by $\langle \nabla f \rangle_2 \equiv \nabla (f * \phi)$. As the kernel ϕ does not depend explicitely on the position, the two approximations $\langle \nabla f \rangle_1$ and $\langle \nabla f \rangle_2$ are equivalent for any regular enough kernel. It is easy to verify that this property is lost when the kernel is position–dependent.

In the applications, to improve spatial resolution the characteristic size of the

kernel is actually allowed to depend on the position and the approximation $\langle \nabla f \rangle_1$ is implicitely applied. In this case the SPH scheme is no longer momentum and energy conservative,[3]. In fact, the use of a position dependent kernel introduces, in the approximation $\langle \nabla f \rangle_1$, a source of error proportional to the characteristic size of the kernel while the approximation of the SPH scheme is of the second order with respect to it, [1].

To overcome this problem, the discrete SPH equations should be modified introducing corrective terms as, for example, deeply discussed in [4]. In [4] it is shown how the inclusion of the proper ∇h terms in the equations of motion leads to significant improvement of energy conservation in cases of SPH simulations of collisions of polytropic spheres.

In this paper we approach this problem in another way trying to answer to the question:

• is it possible to reduce unconservativity within the general order of approximation of SPH without modifying its, appealingly simple, form?

We believe that the use of the approximation $\langle \nabla f \rangle_2$ would be desirable for this, and we will give, in the Appendix, a strong argument in support. Consequently, we simply look for kernels such that the exchange between the approximation $\langle \nabla f \rangle_2$ and $\langle \nabla f \rangle_1$ introduces a negligible error. This approach has the advantage that no changes on the discrete SPH equations are needed.

We stress that the kernels proposed and commonly adopted in SPH, have been selected either following the spline interpolation theory, [5,6], or minimizing the error in the approximation of f with $f * \phi$, [7]. A recent paper, [9], gives a quite complete statistical analysis of the quality of kernels of various types (i.e. shapes) to reproduce the derivatives of given functions sampled on a one-dimensional, even spaced, mesh. Then our analysis is substantially different from all the previous ones. In particular we are not interested here in the topic of selecting the kernel's width as a function of the particle's position, but rather to identify kernels able to keep second order accuracy of SPH as interpolation technique even in the case of position–dependent kernel width.

The plan of the paper is the following: in Section 2 we introduce the kind of kernels we deal with; in Section 3 the interpolation procedure is studied in detail, and we state a general criterion for selecting kernels; in Section 4 some kernels are accordingly proposed; in Section 5, a simple numerical test is performed, while Sect. 6 is devoted to draw the Conclusions.

2 The kernel function

First of all let us define the kernel ϕ to use in the mollification procedure. We shall assume the following general form

$$\phi(\mathbf{r}, h) \propto h^{-n} g(r/h) \tag{1}$$

where $\mathbf{r} = (r_1, r_2, ..., r_n)$ is the position vector in $\Re^n$, $r = |\mathbf{r}|$, $g(x)$ is a smooth scalar function of the real variable x, with $g'(0) \equiv (dg/dx)_{x=0} = 0$ and such that the kernel has finite moments up to a sufficiently high order. The normalization condition $\int \phi \, d\mathbf{r} = 1$ (the integral is extended over all the physical space) for any h value is imposed. Notice that these assumptions ensure that $\sup_{\mathbf{r}} |f*\phi - f| \propto h^2$, for any sufficiently smooth function $f(\mathbf{r})$. This means that the regularized approximating function $f * \phi$ tends uniformly to the "true" function f as h goes to zero. The function g defines the shape of the kernel, which is particularly important when gradients have to be evaluated.

3 A criterion for the kernel choice

In this Section we consider the step of the SPH-like interpolation procedure related to the approximation of derivatives of a function. In particular we study the difference between $(\nabla f) * \phi$ and $\nabla(f * \phi)$ when ϕ depends explicitly on the position. As a result we shall derive a first general criterion for the right choice of the shape of kernels of the type (1).

Before starting our analysis we find convenient to specify the notations adopted hereafter. We define two differential operators,

$$\nabla_{\mathbf{r}} \equiv \left(\frac{d}{dr_1}, \frac{d}{dr_2}, ..., \frac{d}{dr_n} \right), \qquad \partial \equiv \left(\frac{\partial}{\partial r_1}, \frac{\partial}{\partial r_2}, ..., \frac{\partial}{\partial r_n} \right); \tag{2}$$

the first one (also referred to as ∇ when no ambiguity occurs) is the usual gradient operator in $\Re^n$ while the second one is a "partial" gradient operator, in the sense that it deals only with the *explicit* dependence on the spatial variables.

As we have sketched in the Introduction, the basic idea behind the SPH-like method is the approximation of the gradient of a quantity basing on the

knowledge of f on the particle positions, only. This idea relies on that

$$(\nabla f) * \phi = f * \nabla\phi = \nabla(f * \phi),$$

these identities being true only under appropriate boundary conditions for f and ϕ and if $h = const$. When $h = h(\mathbf{r})$ then integration by parts leads to $\nabla(f * \phi) = f * \partial\phi$ and

$$(\nabla f) * \phi \equiv \langle \nabla f \rangle_1 = \int \nabla_{\mathbf{r}'} f(\mathbf{r}')\phi(\mathbf{r} - \mathbf{r}', h(\mathbf{r}))d\mathbf{r}' =$$

$$= \nabla_{\mathbf{r}} \int f(\mathbf{r}')\phi(\mathbf{r} - \mathbf{r}', h(\mathbf{r}))d\mathbf{r}' - \delta = \nabla(f * \phi) - \delta \equiv \langle \nabla f \rangle_2 - \delta, \qquad (3)$$

where δ depends on f and h. In this case, the normalization condition on the kernel implies

$$\int \partial\phi(\mathbf{r} - \mathbf{r}', h(\mathbf{r}))d\mathbf{r}' = 0, \qquad \int \frac{d}{dh}\phi(\mathbf{r} - \mathbf{r}', h(\mathbf{r}))d\mathbf{r}' = 0. \qquad (4)$$

Our aim is now to find how making δ as small as possible independently of f. Taking into account (1), let us evaluate δ:

$$\delta \equiv \int f(\mathbf{r}')\nabla h(\mathbf{r})\frac{d}{dh}\phi(\mathbf{r} - \mathbf{r}', h(\mathbf{r}))d\mathbf{r}' \propto$$

$$-\frac{\nabla h(\mathbf{r})}{h^{n+1}(\mathbf{r})} \int f(\mathbf{r}')[ng(|\mathbf{r} - \mathbf{r}'|/h(\mathbf{r})) + \frac{|\mathbf{r} - \mathbf{r}'|}{h(\mathbf{r})}g'(|\mathbf{r} - \mathbf{r}'|/h(\mathbf{r}))]d\mathbf{r}'. \qquad (5)$$

In order to recover the equality $(\nabla f) * \phi = \nabla(f * \phi)$, independently of f, the function g in (5) should satisfy, in $\Re^+$, the ordinary differential equation

$$ng(x) + xg'(x) = 0. \qquad (6)$$

The non-trivial solution of this ODE is given by $g \propto x^{-n}$, which leads to a non–normalizable kernel. This means that, with a choice of g in the set of normalizable kernels, δ cannot vanish for all functions f.

Thus, a possibility is to minimize δ via its expansion in terms of the parameter h, looking for conditions that allow to eliminate at least some low order terms on h.

Performing a Taylor expansion of the function f up to the second order around the point $\mathbf{r}$, and taking into account the symmetry of the kernel and the

normalizing conditions, it is easy to verify that

$$\delta = \frac{1}{2}\nabla h(\mathbf{r})\Delta f(\mathbf{r}) \int (r_1 - r'_1)^2 \frac{d}{dh}\phi(\mathbf{r} - \mathbf{r}', h(\mathbf{r}))d\mathbf{r}' + \psi(\mathbf{r})O(h^2), \quad (7)$$

where ψ is a function of the position and Δ is the Laplace operator. Now, we look for kernels that minimize the absolute value of the integral in (7). Let us work out the case $n \geq 3$ (the simpler cases $n = 1$ and $n = 2$ must be handled in a slight different way). Making the substitution $\mathbf{z} = (\mathbf{r} - \mathbf{r}')/h(\mathbf{r})$ the integral in (7) can be written as

$$h(\mathbf{r}) \int z_1^2(ng(|\mathbf{z}|) + g'(|\mathbf{z}|)|\mathbf{z}|)d\mathbf{z}. \quad (8)$$

To perform the integral in (8) we introduce the set of cylindrical variables $(z_1, \rho, \theta_3, ..., \theta_n)$, thus getting, after simple manipulations of variables:

$$\frac{1}{2}(n-1)\omega_{n-1} \int_{-\infty}^{\infty} d\rho \int_{-\infty}^{\infty} |\rho|^{n-2} z_1^2 \left[ng(\sqrt{z_1^2 + \rho^2}) + g'(\sqrt{z_1^2 + \rho^2})\sqrt{z_1^2 + \rho^2}\right] dz_1, \quad (9)$$

where ω_n is the volume of the n–dimensional unitary sphere. Moreover, using polar coordinates (α, β) on the plane (z_1, ρ), the expression (9) becomes

$$\frac{1}{2}(n-1)\omega_{n-1} \int_0^{2\pi} sin^2(\beta)|cos(\beta)|d\beta \int_0^{\infty} \alpha^{n+1}(ng(\alpha) + g'(\alpha)\alpha)d\alpha; \quad (10)$$

the normalization condition, now, is

$$\frac{1}{2}(n-1)\omega_{n-1} \int_0^{2\pi} |sin(\beta)|d\beta \int_0^{\infty} g(\alpha)\alpha^{n-1}d\alpha = 1. \quad (11)$$

It is clear that the approximation of $(\nabla f) * \phi$ with $\nabla(f * \phi)$ improves of, at least, one order with respect to h if the normalized kernel has a shape such that the integral over α in (10) is zero. This improvement makes the SPH–like interpolation with variable kernel size of the same order (the second) of the classic SPH interpolation with constant h (see Appendix).

Thus, we get a criterion to select kernels:

kernels of type (1) should be chosen selecting g in the class of differentiable

functions such that

$$\int_0^\infty \alpha^{n+1}(ng(\alpha)+g'(\alpha)\alpha)\,d\alpha = 0 \quad , \quad 0 < \int_0^\infty \alpha^{n-1} g(\alpha) d\alpha < \infty. \tag{12}$$

Remark 1: it is easily shown that also the cases $n = 1$ and $n = 2$ lead to the same constrain (12) for the selection of the kernel. Remark 2: the stated criterion is of course useless if $\nabla h(\mathbf{r})$ is imposed to be zero. Remark 3: this analysis may be iterated by evaluating higher order terms in the Taylor expansion of the interpolated function f, and imposing them to be zero.

As final, relevant, consideration we notice that the shape of our proposed 'optimal ' kernel depends on the dimension, n, of the space ; of course this should be taken into account in the practical applications.

4 Some examples and applications

We want, now, to apply the stated criterion to select kernels (in some specific class of functions) in the most common three–dimensional case. The most used kernels in SPH numerical applications derive from the theory of spline functions, [5,6]. Thus, we consider the class of functions (which corresponds to the third-order spline functions class) defined as:

$$g(r) = \begin{cases} ar^3 + br^2 + cr + d & 0 \le r \le 1 \\ a'r^3 + b'r^2 + c'r + d' & 1 \le r \le 2 \\ 0 & r > 2, \end{cases} \tag{13}$$

continuous up to the second derivative and such that:

(i) $g(0) = 1$ and $g(2) = 0$;
(ii) the first derivative vanishes on the boundary of the set $[0, 2]$.

Following the criterion discussed in Section 3, the selected normalized $3 - D$ kernel in this class is found to be

$$\phi(\mathbf{r}, h) = \frac{15}{1152\pi h^3} \begin{cases} (r/h)^2 \left(171\ (r/h) - 321\right) + 172 & 0 \le r/h \le 1 \\ \left((r/h) - 2\right)^2 \left(107 - 85\ (r/h)\right) & 1 \le r/h \le 2 \\ 0 & r/h > 2. \end{cases} \tag{14}$$

Fig. 1. The kernel (14) selected with our method (solid line) is compared with the kernel (17) (dashed line).

Another kernel often used in the applications belongs to the super-Gaussian class of kernels:

$$g(r) = (ar^2 + b)e^{-r^2} \quad , \quad r \geq 0. \tag{15}$$

When applied to this class of functions, our criterion yields (in $3 - D$)

$$\phi(\mathbf{r}, h) = \frac{1}{\pi^{3/2}h^3}\left(\frac{5}{2} - (r/h)^2\right)e^{-(r/h)^2}. \tag{16}$$

We note that the kernel (14) differs from the kernel belonging to the same class and suggested by Monaghan and Lattanzio [6] (see also Figure 1), i.e.:

$$\phi(\mathbf{r}, h) = \frac{1}{\pi h^3}\begin{cases} 1 - \frac{3}{2}(r/h)^2 + \frac{3}{4}(r/h)^3 & 0 \leq r/h \leq 1 \\ \frac{1}{4}\left(2 - (r/h)\right)^3 & 1 \leq r/h \leq 2 \\ 0 & r/h > 2, \end{cases} \tag{17}$$

On the other hand the kernel (16) is exactly the same super-Gaussian kernel suggested by Gingold and Monaghan [7].

Finally, note that a kernel which is somewhere negative is compatible with our analysis, for we never made assumptions on the sign of g in (1). Nevertheless, a non-negative kernel should be desirable whether the interpolated function is thought to have some specific physical meaning (for example when it represents a mass density). A possible way to overcome this problem could be the use of two different kernels to represent the physical quantities and their gradients separately, but this point should deserve a deeper analysis.

5 A numerical test

The problem of having a good interpolation of derivatives occurs often in the applications and, even if it does not guarantee the quality of SPH evolutive simulations, surely helps in fluid–dynamical numerical simulations.

Of course, when violent shock fronts appear in fluid–dynamical simulations, to keep energy and momentum conservations at a high level of precision requires both a large number of particles in around the front (i.e. high resolution) and modification of SPH equations by mean of the inclusion of the relevant ∇h term, as shown in [4]. Actually, we could check this in an SPH simulation of the classic case of 1-D shock tube calculation, after selecting the best 1-D kernel in the class of cubic splines, following our, previously described, recipe. The treatment of shocks improves with our kernel, but the most significant improvement come actually from higher resolutions and ∇h terms inclusion.

We shall use here our selected kernel (14) in a numerical example of function gradient interpolation, comparing our results with the analogous ones obtained using the kernel (17) suggested by Monaghan and Lattanzio [6] (of course, the 3-D case is by far the most important in practical applications). To this aim, we evaluate numerically the gradient of a function f, supposed known on a set of positions, by SPH-like interpolation. We will perform the test using kernels whose widths strongly depend on the position. To this end we will set the points on a non–uniform grid, and will fix the kernel widths so that only a fixed number of points will be "touched" by any kernel.

The integral $(\nabla f) * \phi \simeq \nabla(f * \phi)$ is then approximated, on the positions $\mathbf{r}_i$, by the Monte-Carlo estimate

$$\frac{1}{N}\sum_{j=1}^{N}\left(\frac{f(\mathbf{r}_j)\partial_{\mathbf{r}}\phi(\mathbf{r}-\mathbf{r}_j,h(\mathbf{r}))}{\rho(\mathbf{r}_j)}\right)_{\mathbf{r}=\mathbf{r}_i}, \qquad i=1,\cdots,N$$

where N is the number of positions $\mathbf{r}_j$ over which f is known and ρ is the number density of the points $\mathbf{r}_j$. As f is assumed to be density of the points, the Monte-Carlo estimate reduces to the simpler form

$$\nabla_{\mathbf{r}} f(\mathbf{r}_i) \sim \frac{1}{N}\sum_{j=1}^{N}\left(\partial_{\mathbf{r}}\phi(\mathbf{r}-\mathbf{r}_j,h(\mathbf{r}))\right)_{\mathbf{r}=\mathbf{r}_i}. \tag{18}$$

In this case, the function f itself is approximated as follows:

$$f(\mathbf{r}_i) \sim \frac{1}{N}\sum_{j=1}^{N}\phi(\mathbf{r}_i-\mathbf{r}_j,h(\mathbf{r}_i)). \tag{19}$$

For the sake of comparison we perform the numerical evaluations using both the kernels (14) and (17).

As "test" function, we choose the function $f(x,y,z) = (2|x-1/2|)^{-1/2}$ in the cube $0 \leq x,y,z \leq 1$, assuming f as point density, too. Being f diverging as $x \to 1/2$, a lot of points $\mathbf{r}_j$ will fall in the neighbourhoud of $x = 1/2$. The exact gradient is $\nabla f(x,y,z) = ((x-1/2)/(2\sqrt{2|x-1/2|^5}), 0, 0)$, singular in $x = 1/2$. Taking into account the meaning of f as a density, the points are displaced on a regular grid. It is easy to verify that the $i_x - th$ position is given by the root of the expression $1 + \sqrt{2} \cdot (x-5)/\sqrt{|x-0.5|} - 2 \cdot i_x/n_x$, where $1 \leq i_x \leq n_x$ and n_x is the number of grid points on the cube edge in the x direction. The setting on the other coordinates is trivial. The total number of grid points is so $n_x \cdot n_y \cdot n_z$. In the test presented here $n_x = 60$ and $n_y = n_z = 50$. The fit to the function and to its gradient have been obtained applying formulas (19) and (18) respectively.

The kernel sizes h are chosen such that for each point the sums (19) and (18) have only 2.5% of non-zero terms, then the size of the kernel depends strongly on the position. That is, the width h changes very rapidly in space. This is surely a situation for which δ, in equation (3), differs from zero: this fact justifies the choice of this particular f.

In Figure 2 the fits obtained with the two cited kernels, along the line $y = z = 1/2$, are presented. Our kernel seems to fits quite better either the function f either the x derivative.

Fig. 2. In Panel (a) the interpolation of the funcion f (solid line) obtained using our kernel (dotted line) and Monaghan and Lattazio's (dashed line) are shown; Panel (b) refers to $\partial f/\partial x$.

As a final consideration, we note that, from a theoretical point af view, the results of this test should depend mainly on the specific dependence of the kernel's widths, $h = h(\mathbf{r})$, with respect to the position, rather than on the particular function, f, chosen for the test.

6 Conclusions

In this paper we have studied an interpolation problem of great interest in practical applications. The problem is the approximation of the derivative of a function, known on a set of points, by a kernel interpolating method. Given a suitable kernel function ϕ, the idea of the method consists in approximating the derivatives of a function f, and so its gradient, with its mollified version $\langle \nabla f \rangle_1 \equiv (\nabla f) * \phi = f * \nabla \phi$, and then evaluating numerically the last convolution integral. This procedure fails as the kernel size depends on the position, i.e. as the operation "$*$" cannot be interpreted as a convolution. In this case, we stated a rule to choose the kernel. The kernel is chosen such to control the difference between $\langle \nabla f \rangle_1$ and the other possible mollification defined as $\langle \nabla f \rangle_2 \equiv \nabla (f * \phi)$ up to a given order in h. This simple criterion is independent of the numerical method applied in the integration. We have given some examples of kernels selected applying our criterion and discussed results in a typical case.

Appendix

Let us consider the evolutive equations for a compressible fluid written in conservative form, [8]:

$$\begin{cases} \rho_t + \nabla_{\mathbf{r}} \cdot \mathbf{q} = 0 \\ q_{it} + \nabla_{\mathbf{r}} \cdot \left(\mathbf{q} \frac{q_i}{\rho} \right) + \nabla_{r_i} P = 0 \qquad i = 1, 2, 3; \\ e_t + \nabla_{\mathbf{r}} \cdot \left[(e + P) \frac{\mathbf{q}}{\rho} \right] = 0, \end{cases} \tag{20}$$

where $\mathbf{q} = \rho \mathbf{v}$ is the density of momentum, P is the pressure, $e/\rho = v^2/2 + \varepsilon$ is the total energy per unit mass and ε is the internal one.

The usual way to get the discrete SPH equations consists in the convolution of each equation with a kernel ϕ and then in its approximation through Monte-Carlo integrations, [1]. We shall consider here the first step only. We begin considering a kernel of the type (1) where h is a constant. The set of equations (20) becomes:

$$\begin{cases} \langle \rho \rangle_t + \nabla_{\mathbf{r}} \cdot \langle \mathbf{q} \rangle = 0 \\ \langle q_i \rangle_t + \nabla_{\mathbf{r}} \cdot \langle \left(\mathbf{q} \frac{q_i}{\rho} \right) \rangle + \nabla_{r_i} \langle P \rangle = 0 \qquad i = 1, 2, 3; \\ \langle e \rangle_t + \nabla_{\mathbf{r}} \cdot \langle \left[(e + P) \frac{\mathbf{q}}{\rho} \right] \rangle = 0, \end{cases} \tag{21}$$

where $\langle \rho \rangle = \int \rho(\mathbf{r}') \phi(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'$, and so on. Let us study the conservation of the mollified quantities. It is straightforward to verify that $\frac{d}{dt} \int \langle \rho \rangle d\mathbf{r} = 0$ and $\int \langle \rho \rangle d\mathbf{r} = \int \rho \, \mathrm{d}\mathbf{r}$, and similar for the other quantities. The conservation of the

mass derives directly by the equation $(\nabla \cdot \mathbf{q}) * \phi = \nabla \cdot (\mathbf{q} * \phi)$ which means (see the Introduction) $\langle \nabla \cdot \mathbf{q} \rangle_1 = \langle \nabla \cdot \mathbf{q} \rangle_2$.

When $h = h(\mathbf{r})$, then $\frac{d}{dt} \int \langle \rho \rangle d\mathbf{r} = O(h)$ and so on (see Section 3); that is the system is not longer conservative and the error derives from the exchange of $(\nabla \cdot \mathbf{q}) * \phi$ with $\nabla \cdot (\mathbf{q} * \phi)$. In other words, the error derives from the exchange of $\langle \nabla \cdot \mathbf{q} \rangle_1$ with $\langle \nabla \cdot \mathbf{q} \rangle_2$. The conclusion is that when the approximation $\langle \nabla f \rangle_2$ cannot be applied, the conservations are lost.

The use of kernels selected on the basis of the criterion stated in Section 3 ensures $\frac{d}{dt} \int \langle \rho \rangle d\mathbf{r} = O(h^2)$, etc..., which is the order of approximation of the SPH method, [3].

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